

1-Hexene
592-41-6 | DTXSID4025402

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.46e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 9.16e-01

Confidence level: 7.48e-01

Nearest Neighbors from the Training Set

Image not found

1-Hexene

Measured: 5.94e-04

Predicted: 6.46e-04

Image not found

Hexene

Measured: 5.94e-04

Predicted: 6.01e-04

Image not found

Methylcyclopentane

Measured: 4.99e-04

Predicted: 6.50e-04

Image not found

4-Methyl-1-pentene

Measured: 5.70e-04

Predicted: 6.65e-04

Image not found

Hept-2-yne

Measured: 1.70e-03

Predicted: 6.94e-04